Class 4: CISD, CCSD and basic DFT

1. Use `rdesktop` to login to the Windows Terminal Server at `minsc.oerc.ox.ac.uk` (use your supercomputer login credentials).
2. Use `ssh` from either the Linux host or from the terminal server to login to `orac.oerc.ox.ac.uk` and load the Gaussian module (`module load gaussian03`).
3. Optimize the geometry of methane at MP2/cc-pVDZ level and compute the energy at the minimum using MP2, MP4, CISD(T), CCSD and CCSD(T) methods. Use `scf=dsymm` to enforce the use of tetrahedral symmetry, otherwise the calculation may take a long time.
4. Optimize glucose geometry using DFT B3LYP/6-31G(d,p) method. Observe the time taken.
5. Compare the hyperfine couplings computed for phenyl neutral radical (benzene without one hydrogen) using RB3LYP/cc-pVDZ, UB3LYP/cc-pVDZ and UB3LYP/EPR-II methods. Comment on the results and compare them to experimental data.
6. Use the redundant coordinate editor in GaussView to set up a potential energy scan with respect to the C-H bond stretch in methane (between 1 and 4 Angstroms). Run the scan using RHF, UHF, RMP2, UMP2, RCCSD, UCCSD, RB3LYP and UB3LYP methods in a cc-pVDZ basis set. Read the logs with GaussView and plot the molecular energy against the stretch parameter. Comment on what you see.

Reminder: ORAC runscripts should look like this

```
#!/bin/bash
#PBS -l ncpus=8
#PBS -l walltime=24:00:00
#PBS -V

cd $PBS_O_WORKDIR
GAUSS_SCRDIR=$TMPDIR
export GAUSS_SCRDIR

g03 ******.com
g03 ******.com
g03 ******.com
```